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Efficient algorithm for generating spectra using line-by-line methods

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Abstract

A method is presented for efficient generation of spectra using line-by-line approaches. The only approximation is replacing the line shape function with an interpolation procedure, which makes the method independent of the line profile functional form. The resulting computational savings for large number of lines is proportional to the number of frequency points in the spectral range. Therefore, for large-scale problems the method can provide speedups of two orders of magnitude or more.

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1. Introduction

Calculations of spectra using line-by-line methods can entail large computational efforts [1]. That is, the spectrum for a configuration-to-configuration transition array is given by,

$$S(\omega) = \sum_{k=1}^{N_\ell} s_k \phi(\omega - \nu_k) \tag{1.1}$$

where $\hbar\omega$ is the photon energy, s_k and ν_k are the strength and center of the kth line respectively, N_ℓ is the number of lines, and $\phi(x)$ is the line profile (identical for all lines in the array) with normalization

$$\int_{-\infty}^{\infty} dx\, \phi(x) = 1 \tag{1.2}$$

The operation count to compute $S(\omega)$ directly from Eq. (1.1) given the atomic data $\{s_k, \nu_k\}$ is

$$N_S \propto O(N_\ell N_\omega N_\phi) \tag{1.3}$$

where N_ω is the number of frequency points and N_ϕ the number of operations to compute ϕ at a given frequency. Since $N_\phi \approx 10$ even for the simple Lorentz profile, $N_\omega = 10^{3-4}$ is typically required in opacity calculations, and configuration-to-configuration transition arrays in low- to mid-Z elements can often have $N_\ell = 10^{5-6}$, evaluation of $S(\omega)$ can take considerable computational effort [1]. Thus, efficient algorithms to generate the spectrum are welcome.

The purpose here is to present a procedure previously implemented in the TOPAZ opacity code [2] that is significantly faster than the explicit calculation of Eq. (1.1) and may benefit the growing number of groups performing line-by-line calculations.

2. Method

The optimized procedure to generate spectra for myriad lines with identical profiles can be separated into three steps: interpolation, line accumulation, and convolution. It is assumed that the spectrum is to be computed on a uniform frequency mesh $\{\omega_i\}$ with $\omega_{i+1} - \omega_i = h$ for all i.

2.1 Interpolation

The first step is to replace explicit evaluation of the profile by interpolation, which is computationally faster and does not significantly compromise accuracy. When many interpolations with the same data set and different arguments must be carried out, the Newton polynomial proves efficient. The line profile and divided-differences are computed on a uniform

detuning mesh $\{x_j\}$ (frequency measured from line center, $x = 0$) with $x_{j+1} - x_j = h$ for all j. Then the interpolation for the profile at a frequency is given by [3]

$$\phi(\omega - \nu_k) = \phi_o[x_j] + \Delta_k \phi_1[x_j, x_{j+1}] + \Delta_k(h - \Delta_k)\phi_2[x_j, x_{j+1}, x_{j+2}] + \cdots \tag{2.1.1}$$

with the divided-differences and k[th] line center displacement from the frequency points given by

$$\phi_n[x_j, \ldots, x_{j+n}] = \begin{cases} \phi_o(x) & , \quad n = 0 \\ \dfrac{\phi_{n-1}[x_{j+1}, \ldots, x_{j+n}] - \phi_{n-1}[x_j, \ldots, x_{j+n-1}]}{x_{j+n} - x_j}, & n \geq 1 \end{cases} \tag{2.1.2}$$

$$\Delta_k = \nu_k - \omega_j \tag{2.1.3}$$

where the index j is defined by

$$x_j < \omega - \nu_k \leq x_{j+1} \tag{2.1.4}$$

and for brevity only terms through second-order were included in Eq. (2.1.1).

2.2 Line accumulation

The second step makes no approximation and involves replacing the sum over lines by a sum over frequencies effectively accumulating the lines. Substitute the results of Section 2.1 into Eq. (1.1) at the grid points $\{\omega_i\}$ to obtain

$$\begin{aligned} S(\omega_i) \approx \tilde{S}(\omega_i) = \sum_{k=1}^{N_\ell} s_k \Big\{ & \phi_o[\omega_i - \omega_j] + \Delta_k \phi_1[\omega_i - \omega_j, \omega_i - \omega_{j+1}] \\ & + \Delta_k(h - \Delta_k)\phi_2[\omega_i - \omega_j, \omega_i - \omega_{j+1}, \omega_i - \omega_{j+2}] \Big\} \end{aligned} \tag{2.2.1}$$

where the index j is now defined by

$$\omega_j < \nu_k \leq \omega_{j+1} \tag{2.2.2}$$

It is possible to write the sum over lines in Eq. (2.2.1) as a sum over frequency points by noting that for a given j all the lines that satisfy Eq. (2.2.2) involve the same ϕ_n coefficients and can be grouped. Thus, Eq. (2.2.1) can be exactly rewritten as

$$\begin{aligned} \tilde{S}(\omega_i) = \sum_{j=1}^{N_\omega} \Big\{ & S_o(\omega_j)\phi_o[\omega_i - \omega_j] + S_1(\omega_j)\phi_1[\omega_i - \omega_j, \omega_i - \omega_{j+1}] \\ & + S_2(\omega_j)\phi_2[\omega_i - \omega_j, \omega_i - \omega_{j+1}, \omega_i - \omega_{j+2}] \Big\} \end{aligned} \tag{2.2.3}$$

where the accumulated quantities are defined by

$$S_o(\omega_j) = \sum_{k=1}^{N_\ell}{}' s_k, \quad S_1(\omega_j) = \sum_{k=1}^{N_\ell}{}' s_k \Delta_k, \quad \text{and} \quad S_2(\omega_j) = \sum_{k=1}^{N_\ell}{}' s_k \Delta_k (h - \Delta_k) \tag{2.2.4}$$

and $\sum'$ denotes a restricted sum satisfying Eq. (2.2.2).

2.3 Convolution

The final step is to recognize the expression in Eq. (2.2.3) as the discrete convolution of the functions S_n and ϕ_n. In terms of indices Eq. (2.2.1) is symbolically

$$\tilde{S}(i) = \sum_{j=1}^{N_\omega} \left\{ S_o(j)\phi_o[i-j] + S_1(j)\phi_1[i-j] + S_2(j)\phi_2[i-j] \right\} \tag{2.3.1}$$

and can be efficiently performed using fast Fourier transform (FFT) methods [4].

2.4 Operation count

The operation count to evaluate the spectrum $S(\omega)$ directly using interpolation is

$$N_S^{\text{int}} \approx O(N_\ell N_\omega N_{\text{int}}) + O(N_\omega N_\phi) \tag{2.4.1}$$

with N_{int} the interpolation operation count rather than explicit calculation (N_ϕ operations) so the second term results from computing the profile and divided differences.

The line accumulation in Eq. (2.2.4) is $O(N_\ell)$ operations. Although explicit convolution is $O(N_\omega^2)$, taking advantage of the FFT methods makes it $O(N_\omega \ln N_\omega)$ [4]. Finally, the operation count for evaluating $S(\omega)$ with the present method is

$$N_S^{FFT} \approx O(N_\ell) + O(N_\omega \ln N_\omega) + O(N_\omega N_\phi) \tag{2.4.2}$$

Comparing the results in Eqs. (2.4.1) and (2.4.2), the speedup is

$$\frac{N_S^{\text{int}}}{N_S^{FFT}} \approx \frac{O(N_\ell N_\omega N_{\text{int}}) + O(N_\omega N_\phi)}{O(N_\ell) + O(N_\omega \ln N_\omega) + O(N_\omega N_\phi)} \tag{2.4.3}$$

which for $N_\omega << N_\ell$ is $O(N_\omega)$ leading to large computational savings.

2.5 Numerical details

There are two situations where the present method can introduce errors that fortunately can be readily evaded. Firstly, if the assumed frequency spacing, h, does not resolve the line profile, then interpolation can be inaccurate near line center. The problem is avoided by using explicit calculation for a few points near line center for each line and implementing the method for the remaining points. Secondly, the FFT methods can produce inaccurate result for values less than about 10^{-12} relative to line center. The termination of the far wing calculations at such a small relative value should not impact the spectrum when continuum processes are included. A matter related to both situations, the far wing might only require linear or even zero order interpolation.

The bound-bound spectrum includes contributions from all configuration-to-configuration transition arrays in a calculation. Some arrays could have $N_\omega >> N_\ell$ for which the present method may not prove advantageous. Such cases, however, do not determine the time of calculation, which is dominated by arrays with large number of lines. Nevertheless, it is sensible to have alternative methods based on estimates of operation counts. This can prevent the computational time from unduly increasing when no transition array has a large number of lines.

A possible extension of the present method is to group lines by similar profiles (e.g.; Lorentz profiles with approximately the same line width). Then apply the method to these larger line sets assuming for each group a representative profile. Although this line-grouping scheme introduces approximations, it could further decrease the computational effort significantly.

6. Conclusion

A method was presented to generate line-by-line spectra efficiently. The first step was to replace the explicit calculation of the profile by the Newton divided-differences interpolating polynomial. The second step is to accumulate the lines effectively reducing their number to the number of frequency points. The final step is recognizing the resulting expression as a convolution and amenable to FFT methods. The reduction in computational effort for a configuration-to-configuration transition array with large number of lines is proportional to the number of frequency points.

The method involves no approximations except for replacing the explicit profile evaluation by interpolation. Specifically, the line accumulation and convolution are exact given the interpolation procedure. Furthermore, the interpolation makes the method independent of the line profile functional form contrary to other schemes using FFT methods to generate line-by-line spectra but relying on the analytic form of the profile Fourier transform [5]. Finally, the method relies on a uniform frequency mesh. For non-uniform frequency meshes, however, the method can be applied by using a suitable temporary uniform mesh and the results interpolated onto the final mesh with little additional cost.

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